Dimethyl glutarate

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 4.51

Global applicability domain: Inside

Local applicability domain index: 9.82e-01

Confidence level: 6.39e-01

Nearest Neighbors from the Training Set

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Propylbenzene
Measured: 4.09
Predicted: 4.53

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Octanal
Measured: 5.36
Predicted: 4.54

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1,2-Dichlorobenzene
Measured: 4.36
Predicted: 4.46

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Hexyl acetate
Measured: 4.58
Predicted: 4.51

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1,3-Dichlorobenzene
Measured: 4.12
Predicted: 4.44